

## Accurate solution for fluid heat flux distribution near a steady state

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1985 J. Phys. A: Math. Gen. 18 2357

(<http://iopscience.iop.org/0305-4470/18/12/032>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 31/05/2010 at 08:54

Please note that [terms and conditions apply](#).

# Accurate solution for fluid heat flux distribution near a steady state

R E Nettleton

University of the Witwatersrand, Johannesburg, South Africa

Received 2 January 1985

**Abstract.** A solution, exact to terms of second order in the temperature gradient,  $\nabla T$ , is obtained to a Fokker-Planck-type equation previously derived for the distribution  $g(\mathbf{v})$  in values  $\mathbf{v}$  of the local heat flux in a large, homogeneous fluid phase. The solution assumes  $\nabla T$  is applied at time  $t=0$ , causing the heat flow to build up and relax toward a steady state. An exact expression for the steady value of  $\langle v^2 \rangle$  is obtained to order  $(\nabla T)^2$  to test an earlier result, obtained by an approximate expansion of  $g$ . The exact solution is more useful than the earlier one, which involved truncation errors, for calculating correlation functions. Relaxing terms in  $g$  are also calculated.

## 1. Introduction

The extended non-equilibrium thermodynamics is concerned with states of a fluid which are sufficiently far from an equilibrium or steady state that both heat flux,  $\mathbf{J}$ , and temperature gradient,  $\nabla T$ , are independent variables (Nettleton 1960, Müller 1967). In this regime, they obey the Cattaneo-Vernotte equation (Cattaneo 1958, Vernotte 1958),

$$\partial \mathbf{J} / \partial t = -2\mu L \mathbf{J} - \gamma \nabla T \quad (1)$$

where  $L$  is a constant or slowly varying function of density and temperature and  $\mu$  is the coefficient in the entropy expansion,  $S = S_0(\rho, T) - \mu \mathbf{J}^2$ , with  $\rho =$  density. If we introduce a distribution function such that  $g(\mathbf{v}) d\mathbf{v}$  is the probability that the heat flux has a value  $\mathbf{v}$  lying in the element  $d\mathbf{v}$ , then  $\mathbf{J}$  is the first moment of  $g$  and (1) the first moment of the equation obeyed by  $g$ .

For the states for which (1) should be valid, a Fokker-Planck-type equation for  $g$  has been derived (Nettleton 1984) from the classical Liouville equation by a projection operator technique of Zwanzig (1960, 1961). This has the form,

$$\partial g / \partial t = \kappa L W(\mathbf{v}) \nabla_{\mathbf{v}}^2 (g / W) + \gamma \nabla_{\mathbf{v}} \cdot \mathbf{g} \cdot \nabla T \quad (2)$$

where  $W(\mathbf{v}) = \int \delta(\mathbf{A}_J(x) - \mathbf{v}) dx$ , and  $\mathbf{A}_J(x)$  is the heat flux operator as a function of phase  $x$ . By finding a solution to (2), it has been possible (Nettleton 1984) to correct the Einstein function  $g \sim \exp[-\mu(\mathbf{v} - \mathbf{J})^2 / \kappa]$  ( $\kappa =$  Boltzmann constant) which has been used to discuss fluctuations from a non-equilibrium state (Jou *et al* 1981). The solution was obtained as a sum of powers and products of  $\mathbf{J} \cdot (\mathbf{v} - \mathbf{J})$ ,  $\nabla T \cdot (\mathbf{v} - \mathbf{J})$ ,  $\mathbf{J}$ , and  $\nabla T$ , with coefficients which are generalised Laguerre polynomials in  $z^2 \equiv (\mu / \kappa)(\mathbf{v} - \mathbf{J})^2$ , starting in zero order with the Einstein function, to which  $g$  must reduce in equilibrium.

When the solution was used to calculate  $\langle(v - \mathbf{J})^2\rangle$ , it appeared that the Einstein function gives the correct result when  $\nabla T = 0$ , but not in the presence of a temperature gradient, in agreement with a kinetic theory result (Jou and Careta 1982).

While the solution to (2) in the form of an expansion in orthogonal polynomials was useful for elucidating the limitations of the Einstein approximation to  $g$ , it could not be used for accurate calculations of correlation functions. To obtain the numerical coefficients of the polynomials, it was necessary to truncate the polynomial expansion, introducing substantial numerical errors into an attempt which was made to calculate  $\langle(v - \mathbf{J})^2\rangle$  to second order in  $\mathbf{J}$  and  $\nabla T$ . To compute more accurate correlation functions and assess the error made in the truncation approximation, we shall proceed in subsequent sections to obtain an exact solution to (2) in which  $W$  is taken to be given by the Gaussian expression assumed previously (Nettleton 1964, 1984). This can be done for the particular case where an external temperature gradient  $\nabla T$  is applied to the system, a small sub-volume immersed in an infinite fluid, at  $t = 0$ , and then held constant so that the system relaxes toward a steady state. In addition to calculating  $\langle v^2 \rangle$  for comparison with the earlier result, we shall be able to demonstrate the existence of the polynomial expansion previously assumed. One can also see that the truncated expansion is not a good representation for very small  $v$  and short times. Since the derivation of (2) with constant  $L$  (Nettleton 1964) fails as  $t \rightarrow 0$ , a solution valid for a time scale over which (1) holds may not be expected to satisfy all physical conditions appropriate to  $t = 0$ .

In § 2, we shall specify the model and assumptions, thus delineating precisely the mathematical problem. In particular, we assume for the solution an expansion in powers of  $\nabla T$ . In § 3, we consider the steady state and obtain in §§ 3.1 and 3.2 an analytic solution for (2) to  $O(\nabla T^2)$ . In § 3.3, the steady-state value of  $\langle v^2 \rangle$  will be compared with the corresponding result from the truncated polynomial expansion, and this will furnish an estimate of the error inherent in the latter. In § 4, additional terms will be calculated which relax exponentially with time. These terms raise questions about the boundary conditions to be applied at  $t = 0$ . A summary and discussion of these points is given in § 5.

## 2. Basic assumptions and description of the problem

The system to be studied is a small sub-volume immersed in a much larger fluid. Since the average heat flow,  $\mathbf{J}$ , in the system is a fast variable which relaxes in a time short compared with the time required for appreciable heat exchange with the surroundings (Jou *et al* 1981), the dynamics of this relaxation (Nettleton 1984) is calculated as for a closed system, from the Liouville equation. The term linear in  $\nabla T$  is then added phenomenologically to (2) to represent the effect of the coupling to the surroundings.  $\nabla T$  characterises the temperature difference between surroundings and system and is not an internal state variable of the latter.

Since the relaxation closely approximates that in a closed system, the entropy is given by the microcanonical expression  $S = \kappa \ln W(\mathbf{J})$ . It is consistent with this, in deriving (1) from the first moment of (2) (Nettleton 1984), to set

$$W(v) \approx C_W \exp(-\mu v^2 / \kappa) \quad (3)$$

which was done in obtaining the orthogonal polynomial solution to (2) and will be done here in obtaining a more exact solution for comparison with the previous one.

Equation (3) has also been used (Nettleton 1964) in deriving phenomenological equations such as (1) from equations of the type of (2). The normalisation constant

$$C_w = \Omega(E)(\mu/\kappa\pi)^{3/2} \quad (4)$$

where  $E$  is the internal energy, which remains approximately constant during relaxation, and  $\Omega(E)$  is the volume of the energy shell of energy  $E$ , over which the  $x$  integrations are taken.

Combining equations (2) and (4), we write the equation to be solved in subsequent sections in the form

$$(\partial/\partial t)(g/W) = \kappa L \nabla_v^2(g/W) + \gamma \nabla_v(g/W) \cdot \nabla T - (2\mu/\kappa)(g/W) \mathbf{v} \cdot \nabla T. \quad (5)$$

For small temperature gradient, the solution can be obtained as a sum of powers of  $\nabla T$ :

$$g/W = \Omega^{-1} + G_1 + G_2 + O(\nabla T^3) \quad (6a)$$

$$G_1 = \mathbf{v} \cdot \nabla T (\hat{G}_1 + \hat{G}_1^t e^{-\lambda t}) \quad (6b)$$

$$G_2 = (\nabla T)^2 (\hat{G}_{21} + \hat{G}_{21}^t e^{-\lambda t} + \hat{G}_{21}^{2t} e^{-2\lambda t} + (\mathbf{v} \cdot \nabla T)^2 (\hat{G}_{22} + \hat{G}_{22}^t e^{-\lambda t} + \hat{G}_{22}^{2t} e^{-2\lambda t})) \quad (6c)$$

where  $G$ ,  $G_1^t$ , and the  $\hat{G}_{ij}$  are functions of  $v$ .  $\lambda = 2\mu L$  so that the first moment of (6b) will agree with the solution,

$$\mathbf{J} = -(\gamma/2\mu L) \nabla T (1 - e^{-\lambda t}), \quad (7)$$

of (1).

If the ansatz defined by (6a)–(6c) is substituted into (5), comparison of terms corresponding to a given power of  $\nabla T$ ,  $\mathbf{v} \cdot \nabla T$ , or  $e^{-\lambda t}$  or product of these yields differential equations which determine  $\hat{G}_1$ ,  $\hat{G}_1^t$ ,  $\hat{G}_{ij}$ , and so on. The time-dependent terms will be taken up in § 4.

### 3. Steady-state solution

We set  $(\partial/\partial t)(g/W) = 0$  in (5) and substitute the  $t \rightarrow \infty$  limits of (6a)–(6c). The resulting solution for  $g$  can be used to calculate  $\langle v^2 \rangle$  to  $O(\nabla T^2)$  for comparison with the result obtained from the earlier (Nettleton 1984) polynomial solution and truncation approximation. We can also establish that, if the solution is to be consistent with (7), the phenomenological Cattaneo–Vernotte equation (1), and a normalisation condition, there must exist weak singularities at  $v \rightarrow 0$ .

#### 3.1. Differential equations and physical conditions

If we substitute the  $t \rightarrow \infty$  limit of (6a)–(6b) into the static limit of (5), we obtain

$$(2/v^2) \hat{G}_1 + (6/v) d\hat{G}_1/dv + d^2 \hat{G}_1/dv^2 = \Gamma \equiv 2\mu\gamma/\kappa^2 \Omega L \quad (8)$$

$$\kappa L [(2/v^2) \hat{G}_{22} + (8/v) d\hat{G}_{22}/dv + d^2 \hat{G}_{22}/dv^2] + (\gamma/v) d\hat{G}_1/dv - (2\mu\gamma/\kappa) \hat{G}_1 = 0 \quad (9)$$

$$\kappa L [(2/v^2) \hat{G}_{21} + (4/v) d\hat{G}_{21}/dv + d^2 \hat{G}_{21}/dv^2 + 2\hat{G}_{22}] + \gamma \hat{G}_1 = 0. \quad (10)$$

These equations can be solved successively and generate six arbitrary constants. Four of these constants are zero if we eschew singular terms  $O(v^{-a})$  with  $a \geq 1$ . The stronger of these must be discarded if  $g(\mathbf{v})$  is to be integrable and expandable in Laguerre polynomials  $L_n^{1/2}(v^2)$  as assumed previously (Nettleton 1984). The remaining

two constants are determined by normalisation and consistency conditions. From the normalisation condition that  $g$  be normalised to unity

$$\int_0^\infty C_w \exp(-\mu v^2/\kappa) G_2 dv = (\nabla T)^2 C_w 4\pi \int_0^\infty \exp(-\mu v^2/\kappa) \times (\hat{G}_{21} + \frac{1}{3}\hat{G}_{22}v^2)v^2 dv = 0. \tag{11}$$

The consistency condition stems from the fact that the first moment of (2) agrees with the Cattaneo-Vernotte equation only if

$$\kappa L(2\mu/\kappa)^2 \langle v v^2 \rangle^{(1)} = 8\mu L \langle v \rangle^{(1)} \tag{12}$$

where  $\langle v \rangle^{(1)}$  is the  $O(\nabla T)$  contribution to  $\langle v \rangle$ . Equation (12) is thus equivalent to the physical arguments used (cf Nettleton 1964) to derive (1) from (2).

### 3.2. Analytic solution

The homogeneous parts of (8)-(10) can be solved by an expression of the form  $v^\rho$ , with  $\rho$  determined in each case by substitution into the equation. To the solutions for the homogeneous parts, we add particular solutions which can be found in a similar way as sums of powers of  $v$ . Thus we find

$$\hat{G}_1 = C'_1 v^{\rho_1} + \frac{1}{16}\Gamma v^2 \tag{13}$$

where  $\rho_1 = \frac{1}{2}[(17)^{1/2} - 5]$ . In line with the discussion in § 3.1, we have discarded a possible term  $v^a$  with  $a = -\frac{1}{2}[(17)^{1/2} + 5] < -4$ . From (12) we establish that

$$C'_1 = -45\Gamma \pi^{1/2} (\kappa/\mu)^{1-\rho_1/2} / [32(\rho_1 + 1)^2(\rho_1 + 3)\Gamma(\frac{1}{2}(\rho_1 + 1))]. \tag{14}$$

On substituting (13) into (9), we find we can solve the latter by methods similar to those applied in (8). The result is

$$\hat{G}_{22} = C_2 v^{\rho_2} + a v^{\rho_1} + b v^2 + c v^{\rho_1+2} + d v^4 \tag{15a}$$

$$a = -(\gamma/2\kappa L) C'_1 \tag{15b}$$

$$b = -\mu\gamma^2/(80\kappa^3\Omega L^2) \tag{15c}$$

$$c = \gamma\mu C'_1/[3(\rho_1 + 3)\kappa^2 L] \tag{15d}$$

$$d = \mu^2\gamma^2/(184\kappa^4\Omega L^2) \tag{15e}$$

$$\rho_2 = \frac{1}{3}[(41)^{1/2} - 7]. \tag{15f}$$

Equations (15a)-(15e) can be used in (10), with the result

$$\hat{G}_{21} = \bar{b} v^{\rho_2+2} + \bar{c} v^{\rho_1+4} + \bar{d} v^4 + \bar{e} v^6 \tag{16a}$$

$$\bar{b} = -C_2/5 \tag{16b}$$

$$\bar{c} = -c/(3\rho_1 + 14) \tag{16c}$$

$$\bar{d} = -\mu\gamma^2/(300\kappa^3\Omega L^2) \tag{16d}$$

$$\bar{e} = -d/28. \tag{16e}$$

The solutions to the homogeneous equation are discarded in (16a) since they are singular and  $O(v^{-1})$  and  $O(v^{-2})$ . Such singularities contradict the structure of  $g$

assumed in deriving phenomenological equations such as (1) from the equation for  $g$  and, when unavoidable, are more likely a consequence of approximations rather than intrinsic physical properties of the system.

The constant  $C_2$  is determined by introducing (15a) and (16a) into (11). We find that

$$C_2(\rho_2 + 3)(\rho_2 + 1)(\kappa/\mu)^{(\rho_2 - 2)/2} \Gamma(\frac{1}{2}(\rho_2 + 1)) = (\mu\gamma^2/\kappa^3\Omega L^2)(15\pi^{1/2}/16)\{-\frac{3}{23} + \frac{2101}{12880} + 5(3\rho_1 + 59)/[16(\rho_1 + 5)]\}. \quad (17)$$

3.3. Static correlation function compared to polynomial result

If we calculate  $\langle v^2 \rangle^{(2)}$ , the  $O(\nabla T^2)$  contribution to the static correlation function,  $\langle v^2 \rangle$ , we obtain

$$\begin{aligned} \langle v^2 \rangle^{(2)} &= 4\pi C_w \int_0^\infty \exp(-\mu v^2/\kappa) (\hat{G}_{21} + \frac{1}{3}\hat{G}_{22}v^2)v^4 dv (\nabla T)^2 \\ &= (\nabla T)^2 (\gamma/\mu L)^2 0.853\ 86. \end{aligned} \quad (18)$$

This is to be compared with the truncated Laguerre polynomial calculation (Nettleton 1984 equation (19)) which  $\langle v^2 \rangle^{(2)} = (\nabla T)^2 (\gamma/\mu L)^2 0.545\ 29$ .

We see that the truncation approximation gives the right order of magnitude but is not accurate. It is useful, therefore, for discussing corrections to, and the domain of validity of, the Einstein approximations as well as for estimating correlations of fluctuations from an arbitrary non-equilibrium state in which  $\mathbf{J}$  and  $\nabla T$  are independently specified. This is a situation more general than that covered by the exact solution developed here.

4. Time-dependent solution

Since the earlier polynomial solution (Nettleton 1984) had terms involving powers of  $\mathbf{J}$ , and  $\mathbf{J}$  has a relaxing contribution  $e^{-\lambda t}$ , we should expect  $G_1$  to have a contribution linear in  $e^{-\lambda t}$ , while  $G_2$  has terms both linear and quadratic, corresponding to terms  $O(J^2)$  and  $O(\mathbf{J} \cdot \nabla T)$  in the earlier solution. These relaxing contributions are embodied in the expressions given in (6b), (6c). In the present section, we substitute (6a)-(6c) into (5) without taking the static limit  $\partial/\partial t(g/W) = 0$ , and compare terms of corresponding order in powers and products of  $e^{-\lambda t}$  and  $\nabla T$  to obtain differential equations for  $\hat{G}'_1$ ,  $\hat{G}'_{2j}$ , and  $\hat{G}'_{2j}$  ( $j = 1, 2$ ).

4.1. Contribution to  $G_1$

On substituting (6b) into (5), we find by comparing terms proportional to  $\mathbf{v} \cdot \nabla T e^{-\lambda t}$  that

$$\kappa L [(2/v^2)\hat{G}'_1 + (6/v) d\hat{G}'_1/dv + d^2\hat{G}'_1/dv^2] + \lambda \hat{G}'_1 = 0. \quad (19)$$

This equation has the solution (Kamke 1948, p 440]

$$\hat{G}'_1 = C_{1t} \chi^{-5/2} J_{\bar{\nu}}(\chi) \quad (20)$$

where  $\chi \equiv (2\mu/\kappa)^{1/2} v$ ,  $\bar{\nu} \equiv \frac{1}{2}(17)^{1/2}$ , and  $J_{\bar{\nu}}$  is a Bessel function of the first kind. The solution with  $J_{\bar{\nu}} \rightarrow J_{-\bar{\nu}}$  is dropped, since it would introduce a non-integrable singularity at  $v \rightarrow 0$ .

The constant  $C_{1t}$  is determined to make the relaxing term in  $\mathbf{J} = \langle \mathbf{v} \rangle^{(1)}$  agree with (7), i.e.

$$\begin{aligned} (4\pi/3)C_w \int_0^\infty \exp(-\mu v^2/\kappa) \hat{G}'_1 v^4 dv \\ = C_{1t} 2^{-5/2} (4\pi/3) C_w \int_0^\infty e^{-\chi^2/2} \chi^{3/2} J_{\bar{\nu}}(\chi) d\chi \\ = \gamma/2\mu L. \end{aligned} \tag{21}$$

The integral in this equation can be evaluated in the form:

$$\begin{aligned} \int_0^\infty e^{-\chi^2/2} \chi^{3/2} J_{\bar{\nu}}(\chi) d\chi \\ = [\Gamma(\frac{1}{2}\bar{\nu} + \frac{5}{4}) / (2^{\bar{\nu}/2 - (1/4)} \Gamma(\bar{\nu} + 1))] {}_1F_1(\frac{1}{2}\bar{\nu} + \frac{5}{4}; \bar{\nu} + 1; -\frac{1}{2}) \end{aligned} \tag{22}$$

${}_1F_1$  is the generalised hypergeometric function (Erdélyi 1953, vol 1, p 182).

#### 4.2. Relaxing components of $G_2$

The equations obtained by comparing terms proportional to  $(\mathbf{v} \cdot \nabla T)^2 e^{-\lambda t}$  and  $(\mathbf{v} \cdot \nabla T)^2 e^{-2\lambda t}$  are, respectively

$$\lambda \hat{G}'_{22} + \kappa L [(2/v^2) \hat{G}'_{22} + (8/v) d\hat{G}'_{22}/dv + d^2 \hat{G}'_{22}/dv^2] + (\gamma/v) d\hat{G}'_1/dv - (2\mu\gamma/\kappa) \hat{G}'_1 = 0 \tag{23a}$$

$$2\lambda \hat{G}^{2t}_{22} + \kappa L [(2/v^2) \hat{G}^{2t}_{22} + (8/v) d\hat{G}^{2t}_{22}/dv + d^2 \hat{G}^{2t}_{22}/dv^2] = 0. \tag{23b}$$

The solution to (23b) and the homogeneous part of (23a) is

$$\phi_{\pm 1}(\chi) = \chi^{-7/2} J_{\pm \nu}(\chi), \quad \nu \equiv \frac{1}{2}(41)^{1/2} \tag{24}$$

so that we have immediately

$$\hat{G}^{2t}_{22} = C^{2t}_{22} \chi^{-7/2} J_\nu(2^{1/2} \chi). \tag{25}$$

We have discarded an unintegrable singularity which would arise from inclusion of the second solution, proportional to  $J_{-\nu}$ .

In addition to a term of the type given by (25),  $\hat{G}^{2t}_{22}$  has an additional term, representing a particular solution of the inhomogeneous (23a). We can write this equation in the form

$$d^2 \hat{G}^{2t}_{22}/d\chi^2 + (8/\chi) d\hat{G}^{2t}_{22}/d\chi + 2\hat{G}^{2t}_{22}(\frac{1}{2} + \chi^{-2}) = h(\chi) \tag{26a}$$

$$h(\chi) = -\gamma C_{1t} \chi^{-5/2} \{ \chi^{-1} J_{\bar{\nu}-1}(\chi) - J_{\bar{\nu}}(\chi) [1 + \chi^{-2}(\frac{5}{2} + \bar{\nu})] \}. \tag{26b}$$

A particular solution to (26a) can be constructed (Kamke 1984, p 117) in the form

$$y_1(\chi) = \phi_{-1} \int W^{-1} \phi_1 h d\chi - \phi_1 \int W^{-1} \phi_{-1} h d\chi \tag{27a}$$

$$W \equiv \phi_1 \phi'_{-1} - \phi'_1 \phi_{-1} = -(2/\pi) \chi^{-8} \sin(\nu\pi). \tag{27b}$$

Substituting from (24) and (26b) into (27a), we calculate

$$\begin{aligned}
 y_1(\chi) &= \chi^{-7/2} J_{-\nu}(\chi) \pi (\sin \nu \pi)^{-1} \gamma C_{1t} [(\nu + \bar{\nu} + 1) \Gamma(\nu + 1) \Gamma(\bar{\nu} + 1) 2^{\nu + \bar{\nu} + 1}]^{-1} \\
 &\quad \times \chi^{\nu + \bar{\nu} + 1} \left\{ -\left(\frac{\xi}{2} + \bar{\nu}\right) {}_3F_4\left(\frac{1}{2}(\nu + \bar{\nu}) + 1, \frac{1}{2}(\nu + \bar{\nu} + 1), \frac{1}{2}(\nu + \bar{\nu} + 1); \nu + 1, \right. \right. \\
 &\quad \times \bar{\nu} + 1, \nu + \bar{\nu} + 1, \frac{1}{2}(\nu + \bar{\nu} + 3); -\chi^2) + 2\bar{\nu} {}_3F_4\left(\frac{1}{2}(\nu + \bar{\nu} + 1), \right. \\
 &\quad \times \frac{1}{2}(\nu + \bar{\nu}), \frac{1}{2}(\nu + \bar{\nu} + 1); \nu + 1, \bar{\nu}, \nu + \bar{\nu}, \frac{1}{2}(\nu + \bar{\nu} + 3); -\chi^2) \\
 &\quad \left. - (\nu + \bar{\nu} + 1)(\nu + \bar{\nu} + 3)^{-1} \chi^2 {}_3F_4\left(\frac{1}{2}(\nu + \bar{\nu}) + 1, \frac{1}{2}(\nu + \bar{\nu} + 1), \right. \right. \\
 &\quad \times \frac{1}{2}(\nu + \bar{\nu} + 3); \nu + 1, \bar{\nu} + 1, \nu + \bar{\nu} + 1, \frac{1}{2}(\nu + \bar{\nu} + 5); -\chi^2) \left. \right\} - (\nu \rightarrow -\nu) \quad (28a) \\
 \hat{G}_{22}^t &= C_{22}^t \chi^{-7/2} J_{\nu}(\chi) + y_1(\chi). \quad (28b)
 \end{aligned}$$

From comparison of terms proportional to  $(\nabla T)^2 e^{-\lambda t}$  and  $(\nabla T)^2 e^{-2\lambda t}$ , we have, respectively:

$$\lambda \hat{G}_{21}^t + \kappa L [2\hat{G}_{22}^t + (2/v^2)\hat{G}_{21}^t + (4/v) d\hat{G}_{21}^t/dv + d^2\hat{G}_{21}^t/dv^2] + \gamma \hat{G}_1^t = 0 \quad (29a)$$

$$2\lambda \hat{G}_{21}^t + \kappa L [2\hat{G}_{22}^t + (2/v^2)G_{21}^t + (4/v) d\hat{G}_{21}^t/dv + d^2\hat{G}_{21}^t/dv^2] = 0. \quad (29b)$$

By methods similar to those employed in calculating  $\hat{G}_{22}^t$ , with a particular solution calculated as in (27a), we obtain

$$\hat{G}_{21}^t = C_{21}^t \chi^{-3/2} J_{\bar{\nu}}(2^{1/2}\chi) + y_2(\chi), \quad \bar{\nu} = \frac{1}{2} \quad (30a)$$

$$\begin{aligned}
 y_2(\chi) &\equiv -\pi(\kappa/\mu) 2^{3/4} C_{22}^t \chi^{-3/2} J_{-\bar{\nu}}(2^{1/2}\chi) \left\{ \chi(2^{1/2}/10)(J_{\bar{\nu}-1}(2^{1/2}\chi) J_{\nu}(2^{1/2}\chi) \right. \\
 &\quad \left. - J_{\bar{\nu}}(2^{1/2}\chi) J_{\nu-1}(2^{1/2}\chi)) + (\bar{\nu} + \nu)^{-1} J_{\bar{\nu}}(2^{1/2}\chi) J_{\nu}(2^{1/2}\chi) \right\} - (\bar{\nu} \rightarrow -\bar{\nu}) \quad (30b)
 \end{aligned}$$

$$\hat{G}_{21}^t = C_{21}^t \chi^{-3/2} J_{\bar{\nu}}(\chi) + y_3(\chi) \quad (31a)$$

$$\begin{aligned}
 y_3(\chi) &= (\pi/\mu) \chi^{-3/2} \sum_{\bar{\nu}=1/2} (2\bar{\nu}) J_{-\bar{\nu}} \left( (\gamma/4L) C_{1t} [\Gamma(\bar{\nu} + 1) \Gamma(\bar{\nu} + 1) 2^{\bar{\nu} + \bar{\nu}} (\nu + \bar{\nu} + 1)]^{-1} \right. \\
 &\quad \times \chi^{\bar{\nu} + \bar{\nu} + 1} {}_3F_4\left(\frac{1}{2}(\bar{\nu} + \bar{\nu}) + 1, \frac{1}{2}(\bar{\nu} + \bar{\nu} + 1), \frac{1}{2}(\bar{\nu} + \bar{\nu} + 1); \bar{\nu} + 1, \bar{\nu} + 1, \bar{\nu} + \bar{\nu} + 1, \right. \\
 &\quad \times \frac{1}{2}(\bar{\nu} + \bar{\nu} + 3); -\chi^2) + \frac{1}{2} \kappa C_{22}^t [(\bar{\nu}^2 - \nu^2)^{-1} \chi \\
 &\quad \times (J_{\bar{\nu}-1}(\chi) J_{\nu}(\chi) - J_{\bar{\nu}}(\chi) J_{\nu-1}(\chi)) - (\bar{\nu} + \nu)^{-1} J_{\bar{\nu}}(\chi) J_{\nu}(\chi)] \\
 &\quad \left. + \frac{1}{4} \kappa \sum_{\pm \nu} \pi \gamma C_{1t} [\sin(\nu \pi)]^{-1} [\Gamma(\nu + 1) \Gamma(\bar{\nu} + 1) 2^{\bar{\nu} + \bar{\nu}} (\nu + \bar{\nu} + 1)]^{-1} \right. \\
 &\quad \times \sum_{m=\infty}^{\infty} 2^{-2m} (m!)^{-1} (-)^m \Gamma(\bar{\nu} - \nu + 2m + 1) [(\bar{\nu} + \bar{\nu} + 2m + 1) \Gamma(\bar{\nu} + m + 1) \\
 &\quad \times \Gamma(-\nu + m + 1) \Gamma(\bar{\nu} - \nu + m + 1)]^{-1} \chi^{\bar{\nu} + \bar{\nu} + 2m + 1} \\
 &\quad \times \left\{ -\left(\frac{\xi}{2} + \bar{\nu}\right) {}_4F_5\left(\frac{1}{2}(\nu + \bar{\nu}) + 1, \frac{1}{2}(\nu + \bar{\nu} + 1), \frac{1}{2}(\nu + \bar{\nu} + 1), m + \frac{1}{2}(\bar{\nu} + \bar{\nu} + 1); \right. \right. \\
 &\quad \times \nu + 1, \bar{\nu} + 1, \nu + \bar{\nu} + 1, \frac{1}{2}(\nu + \bar{\nu} + 3), m + \frac{1}{2}(\bar{\nu} + \bar{\nu} + 3); -\chi^2) \\
 &\quad \left. + 2\bar{\nu} {}_4F_5\left(\frac{1}{2}(\nu + \bar{\nu} + 1), \frac{1}{2}(\nu + \bar{\nu}), \frac{1}{2}(\nu + \bar{\nu} + 1), m + \frac{1}{2}(\bar{\nu} + \bar{\nu} + 1); \right. \right. \\
 &\quad \times \nu + 1, \bar{\nu}, \nu + \bar{\nu}, \frac{1}{2}(\nu + \bar{\nu} + 3), m + \frac{1}{2}(\bar{\nu} + \bar{\nu} + 3) \\
 &\quad \left. + (\bar{\nu} + \bar{\nu} + 2m + 1)(\nu + \bar{\nu} + 1) [(\bar{\nu} + \bar{\nu} + 2m + 3)(\nu + \bar{\nu} + 3)]^{-1} \right. \\
 &\quad \times \chi^2 {}_4F_5\left(\frac{1}{2}(\nu + \bar{\nu}) + 1, \frac{1}{2}(\nu + \bar{\nu} + 1), \frac{1}{2}(\nu + \bar{\nu} + 3), m + \frac{1}{2}(\bar{\nu} + \bar{\nu} + 3); \right. \\
 &\quad \left. \left. \times \nu + 1, \bar{\nu} + 1, \nu + \bar{\nu} + 1, \frac{1}{2}(\nu + \bar{\nu} + 5), m + \frac{1}{2}(\bar{\nu} + \bar{\nu} + 5); -\chi^2) \right\}. \quad (31b)
 \end{aligned}$$



The four constants,  $C_{21}^t$ ,  $C_{21}^{2t}$ ,  $C_{22}^t$ , and  $C_{22}^{2t}$ , are to be determined by the normalisation and boundary conditions. The normalisation of  $g$  to unity requires that

$$\int_0^\infty \exp(-\mu v^2/\kappa) (\hat{G}_{21}^t + \frac{1}{3} \hat{G}_{22}^t v^2) v^2 dv = 0$$

$$= \int_0^\infty \exp(-\mu v^2/\kappa) (\hat{G}_{21}^{2t} + \frac{1}{3} \hat{G}_{22}^{2t} v^2) v^2 dv. \tag{32}$$

A boundary condition sufficient to determine the remaining two constants is provided by inertia, which prevents any instantaneous response, i.e.

$$\langle \mathbf{v}\mathbf{v} \rangle^{(2)} = 0 \quad \text{when } t = 0. \tag{33}$$

This tensor equation has two independent components, e.g.  $\langle v_1 v_1 \rangle^{(2)}$  and  $\langle v_3 v_3 \rangle^{(2)}$ , where  $v_3$  is the component along  $\nabla T$ .

If we apply condition (33), then  $C_{21}^t$  and  $C_{21}^{2t}$  cannot vanish, and  $\hat{G}_{21}^t$ ,  $\hat{G}_{21}^{2t}$  have singularities  $O(v^{-1})$ . These are integrable and can be expanded in infinite sums of generalised Laguerre polynomials  $L_n^{(1/2)}(v^2)$ . Therefore, there is no inconsistency with the assumptions of the earlier work (Nettleton 1984). However, the polynomial sum converges slowly as  $v \rightarrow 0$ . It must be remembered that (2) with constant  $L$  is no longer valid as  $t \rightarrow 0$ , since  $L$  (Nettleton 1964) is a correlation function which becomes time-dependent for small  $t$ . Therefore, it would be equally reasonable to eschew  $O(v^{-1})$  singularities, set  $C_{21}^t = 0 = C_{21}^{2t}$ , and impose no inertial requirement on the higher moments of  $g$  at  $t = 0$ , since the expression on which we seek to impose such a condition is valid only at longer times, when (1) holds. Under these circumstances, since  $y_2(\chi)$  and  $y_3(\chi)$  are not singular as  $v \rightarrow 0$ , and the remaining terms in  $g$  to  $O(\nabla T^2)$  do not become infinite at  $t = 0$  when we take into account the factors  $\mathbf{v} \cdot \nabla T$  and  $(\mathbf{v} \cdot \nabla T)^2$ ,  $g$  will have no infinities. The existence of infinities is an indication of an invalid extension of (2) and (5) into a time domain where they no longer apply.

### 5. Summary and discussion

In earlier work (Nettleton 1964) it was demonstrated that, with the aid of a projection operator proposed by Zwanzig (1960, 1961), one can derive from the classical Liouville equation a Fokker-Planck-type equation for the distribution  $g$  of fluctuations of the thermodynamic variables from their averages in a time-dependent ensemble. This can be done for the case where the variables include the heat flux or time derivatives of structural parameters, so that we are in the domain of extended non-equilibrium thermodynamics. This formalism has been applied (Nettleton 1984) to calculate the distribution  $g(v)$  of values  $v$  of the average heat flux through a small sub-volume immersed in a much larger fluid. The calculation assumes an arbitrary non-equilibrium state, with  $\mathbf{J} = \langle \mathbf{v} \rangle$  and  $\nabla T$  prescribed independently and the solution is obtained as a sum of powers of  $\mathbf{J}$ ,  $\nabla T$ ,  $\mathbf{v}$ , and scalar products thereof with coefficients which are sums of generalised Laguerre polynomials  $L_n^{(1/2)}(z^2)$ ,  $\mathbf{z} \equiv (\mu/\kappa)^{1/2}(\mathbf{v} - \mathbf{J})$ .

The expansion in Laguerre polynomials permits us to discuss fluctuations from an arbitrary state, which is more general than the case considered in the present paper where the system relaxes toward a steady state, induced by constant  $\nabla T$  applied at  $t = 0$ . However, to calculate the numerical coefficients in the polynomial expansion, it was necessary to truncate the latter, leading to errors whose magnitude could not

be assessed without an exact solution to (5) for  $g$  of the kind obtained in the present paper. When the present solution is used to calculate the  $O(\nabla T^2)$  contribution to  $\langle v^2 \rangle$ , and this is compared with the earlier result, we find there is order-of-magnitude agreement only, so that the polynomial expansion is useful only for discussing the validity of the Einstein approximation to  $g$  and the form and magnitude of corrections to it, but a more accurate solution for  $g$  is required if we seek to calculate correlation functions.

A problem arises when it comes to calculating a time-dependent solution from the circumstance that (2) was derived with a view to predicting (1) from its first moment. Therefore (2) and (5), with constant  $L$ , are only valid for times when (1) holds and not as  $t \rightarrow 0$ . In the latter limit  $L$ , which is a time correlation over time  $t$  (Nettleton 1964, cf (33)), is time-dependent. Therefore, it is not entirely consistent to apply a boundary condition such as (33). The latter should hold if the solution were physically exact as  $t \rightarrow 0$ , since otherwise there is an instantaneous response. However, we have seen in § 4.2 that infinities  $O(v^{-1})$  appear in  $\hat{G}_{21}^t$  and  $\hat{G}_{21}^{2t}$  if (33) is imposed, and their origin is most likely related to the unphysical nature of the solution in the  $t \rightarrow 0$  limit. We can remove the infinities by setting  $C_{21}^t = 0 = C_{21}^{2t}$ , causing the higher moments of  $g$ , but not the first moment, to exhibit an instantaneous response as  $t \rightarrow 0$ . The correlation functions are then expected to be correct at longer times, where the assumptions behind (2) and (5) can be justified and, in particular, as  $t \rightarrow 0$ . We should be able, therefore, to use the solution calculated in §§ 3 and 4 in the extended non-equilibrium thermodynamic regime and in the static limit.

While the exact solution can be obtained in a form which has no infinities, still we see from (13), (15a), (25) and (28b) that there are weak singularities  $O(v^{-a})$ , where  $a < \frac{1}{2}$  as  $v \rightarrow 0$ . Such a function can be expanded in polynomials  $L_n^{(1/2)}(v^2)$ , although truncation fails for small  $v$ . Accordingly, the only contradiction with the assumptions of the polynomial solution of (5) is to call in question the numerical accuracy of any low-order truncation of the expansion.

## References

- Cattaneo C 1958 *C.R. Acad. Sci., Paris* **247** 431  
 Erdélyi A (ed) 1953 *Higher Transcendental Functions* (New York: McGraw-Hill)  
 Jou D and Careta T 1982 *J. Phys. A: Math. Gen.* **15** 3195  
 Jou D, Llebot J E and Casas-Vazquez J 1981 *Physica* **109A** 208  
 Kamke E 1948 *Differentialgleichungen Lösungsmethoden und Lösungen* (New York: Chelsea)  
 Müller I 1967 *Z. Phys.* **198** 329  
 Nettleton R E 1960 *Phys. Fluids* **3** 216  
 — 1964 *J. Chem. Phys.* **40** 112  
 — 1984 *J. Phys. A: Math. Gen.* **17** 2149  
 Vernotte P 1958 *C.R. Acad. Sci., Paris* **247** 3154  
 Zwanzig R 1960 *J. Chem. Phys.* **33** 1338  
 — 1961 *Phys. Rev.* **124** 983